Gluconolactone

## Model Performance

| Model | Data |
|---|---|

### Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|---|---|---|---|---|---|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

## Model Results

**Predicted value:** 2.47e-10 mmHg

**Global applicability domain:** Inside

**Local applicability domain index:** 3.50e-01

**Confidence level:** 2.79e-01

## Nearest Neighbors from the Training Set

Image not found

2,2,5,5-Tetramethylhexane
**Measured:** 9.80e-08
**Predicted:** 7.94

Image not found

Benz(a)anthracene
**Measured:** 1.97e-10
**Predicted:** 2.14e-08

Image not found

Lepidine
**Measured:** 8.02e-14
**Predicted:** 9.90e-03

Image not found

Perflutren
**Measured:** 1.66e-08
**Predicted:** 7890

Image not found

Dibenzofuran, 1,2,3,4,8-
pentachloro-
**Measured:** 2.84e-11
**Predicted:** 2.10e-09